Quantum Transition from Order to Chaos in the Nuclear Shell Model [1]

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Abstract. We discuss the role of quantum chaos in atomic nuclei. After reviewing the basic assumptions of the nuclear shell model, we analyze the spectral statistics of the energy levels obtained with realistic shell–model calculations in the fp shell. In particular, for Ca isotopes we observe a transition from order to chaos by increasing the excitation energy and a clear quantum signature of the breaking of integrability by changing the single–particle spacings.

1 Chaos and Quantum Chaos

Quantum chaos is the study of the properties of quantal systems which are classically chaotic, thus with exponential divergence of initially closed trajectories in the phase space [1].

The energy fluctuation properties of systems with underlying classical chaotic behaviour and time–reversal symmetry agree with the predictions of the Gaussian Orthogonal Ensemble (GOE) of random matrix theory, whereas quantum analogs of classically integrable systems display the characteristics of the Poisson statistics [2].

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The most used quantity to study the local fluctuations of the energy levels is the spectral statistics $P(s)$. $P(s)$ is the distribution of nearest–neighbour spacings $s_i = (\tilde{E}_{i+1} - \tilde{E}_i)$ of the unfolded levels $\tilde{E}_i$. It is obtained by accumulating the number of spacings that lie within the bin $(s, s+\Delta s)$ and then normalizing $P(s)$ to unity. For quantum systems whose classical analogs are integrable, $P(s)$ is expected to follow the Poisson limit, i.e. $P(s) = \exp(-s)$. On the other hand, quantal analogs of chaotic systems exhibit the spectral properties of GOE with $P(s) = (\pi/2)s\exp(-\frac{\pi}{4}s^2)$, which is the so–called Wigner distribution. The distribution $P(s)$ is the best spectral statistics to analyze shorter series of energy levels and intermediate regions between order and chaos [1,2].

2 The Nuclear Shell Model

One of the best systems for the study of quantum chaos is the atomic nucleus. In fact, its experimental energy levels have been studied in the domain of neutron and proton resonances near the nucleon emission threshold, where a large number of levels with the same spin and parity in the same nucleus are present, and an excellent agreement with GOE predictions has been found [3].

In the nuclear shell model [4], the nuclear states, like the electronic states in atoms, are described in terms of the motion of nucleons in a mean–field. But, while the nuclear field is generated by the interactions of the nucleons (protons and neutrons), the atomic field is mainly governed by the interaction of the electrons with the nucleus.

The Hamiltonian of the shell model can be written as:

$$H_0 = \sum_{i=1}^{A} \Big(-\frac{\hbar^2}{2m_i}\nabla_i^2 + U_i \Big) \; , \qquad (1)$$

where A is the number of nucleons, m_i is the mass of the i-th nucleon, and U_i is the mean–field. The choice of the mean–field is crucial; U_i may be obtained by the usual methods using the many body theory [4].

To obtain a good agreement between the shell model results and the experimental data, it is necessary to add a residual interaction H_R so that the total hamiltonian H can be written:

$$H = H_0 + H_R \; , \qquad (2)$$

where H_R is the part of nucleon–nucleon interaction not included in H_0. Using second quantization formalism [4], we can write:

$$H_0 = \sum_{\alpha} \epsilon_\alpha a_\alpha^+ a_\alpha \ , \tag{3}$$

$$H_R = \sum_{\alpha\beta\gamma\delta} < \alpha\beta|V|\delta\gamma > a_\alpha^+ a_\beta^+ a_\gamma a_\delta \ , \tag{4}$$

where the labels denote the accessible single–particle states, ϵ_α is the corresponding single–particle energy, and $< \alpha\beta|V|\delta\gamma >$ is the two–body matrix element of the nuclear residual interaction. The operators a_α^+ and a_α are the fermionic creation and annihilation operators of the α–th single nucleon state and H_R can be calculated by the Hartree–Fock equations, starting from the free nucleon interactions. Many nucleons are frozen in the deeper shells of the mean field potential and form an inert core; only a few nucleons partially populate the single particle shells outside the core. These are called valence–nucleons. So there are N valence–nucleons, m active shells and a finite number of energy levels. It is standard procedure to cut the basis states by introducing a finite number of configurations which are sufficient to describe the first excitation states [4].

3 Spectral Statistics and the Brody Distribution

We study the ($f_{7/2}$,$p_{3/2}$,$f_{5/2}$,$p_{1/2}$) shell–model space, assuming ^{40}Ca as an inert core with $4 < N < 10$ valence–nucleons. The diagonalizations are performed by using Lanczos and Householder algorithms with the code ANTOINE [5,6]. For a fixed number of valence protons and neutrons we calculate the energy spectrum for total angular momentum J and total isospin T. The single–particle energies (in MeV) are $\epsilon_{7/2} = 0$, $\epsilon_{3/2} = 2$, $\epsilon_{1/2} = 4$ and $\epsilon_{5/2} = 6.5$. The residual interaction we use is a minimally modified Kuo–Brown realistic force with monopole improvements [6].

For the low–lying levels, the spectrum is mapped onto unfolded levels with quasi–uniform level density by using both the constant temperature formula [7] and the local unfolding method [8]. The two procedures give the same results. For the full spectrum we use the local unfolding because

the constant temperature formula is valid only when the level density grows exponentially.

To quantify the chaoticity of the distribution $P(s)$ (nearest–neighbour spacings of the energy levels) in terms of a parameter, we compare it to the Brody distribution

$$P(s,\omega) = \alpha(\omega+1)s^{\omega} \exp\left(-\alpha s^{\omega+1}\right) , \tag{5}$$

with

$$\alpha = (\Gamma[\frac{\omega+2}{\omega+1}])^{\omega+1} . \tag{6}$$

This distribution interpolates between the Poisson distribution ($\omega = 0$) of regular systems and the Wigner distribution ($\omega = 1$) of chaotic ones (GOE). The parameter ω can be used as a simple quantitative measure of the degree of chaoticity [9].

Table 1. Brody parameter ω for Ca isotopes.

^{44}Ca	^{45}Ca	^{46}Ca	^{47}Ca	^{48}Ca	^{49}Ca	^{50}Ca
0.69	0.75	0.99	0.98	0.95	1.00	0.87

Table 1 shows the Brody parameter ω for the whole spectrum of the analyzed Ca isoptopes (only neutrons in the fp shell), which range from ^{44}Ca to ^{50}Ca. We see that only the lightest Ca isotopes are not fully chaotic.

It now becomes interesting to analyze the Brody parameter as a function of the excitation energy. We calculate the $P(s)$ distribution and the Brody parameter up to a fixed value of the excitation energy above the yrast lines. Obviously this cannot be done for the lightest Ca isotopes because few levels are involved.

Table 2. Brody parameter ω as a function the the Energy for Ca isotopes.

Energy (MeV)	^{48}Ca	^{49}Ca	^{50}Ca
6	0.54	0.63	0.72
8	0.65	0.70	0.79
10	0.78	0.81	0.84
12	0.83	0.82	0.86
14	0.90	0.86	0.88
16	0.87	0.92	0.90
18	0.93	0.95	0.92

The results are written in Table 2 for ^{48}Ca, ^{49}Ca and ^{50}Ca and show a strong energy dependence: there is an order–chaos transition by increasing the excitation energy.

Another important aspect is the effect of the one–body Hamiltonian on the two–body residual interaction when the single–particle spacings are changed.

Table 3. Brody parameter ω for Ca isotopes.

Single Particle Spacings	^{44}Ca	^{45}Ca
degenerate	0.85	0.98
normal	0.69	0.75
double–spaced	0.29	0.58

Table 3 shows that with degenerate single–particle levels the isotopes ^{44}Ca and ^{45}Ca are chaotic while for double–spaced single–particle levels they are quasi–regular. This interesting effect is a clear quantum signature of the breaking of the integrability due to the residual interaction. In fact, the one–body Hamiltonian is classically integrable because it is the sum of harmonic oscillators while the two–body residual interaction is strongly non–linear. By increasing the single–particle spacings, the single–particle mean–field motion in the valence orbits suffers less disturbance and is thus more regular.

4 Summary

We have studied quantum chaos in atomic nuclei by using the nuclear shell model. We have calculated the spectral statistics of Ca isotopes by using Lanczos and Householder algorithms with the shell–model code ANTOINE. The Brody parameter, which fits the nearest–neighbour spacings distribution of the energy levels, shows an order–chaos transition when the excitation energy is increased and when the single–particle spacings are changed.

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